User Suggestions and
State of Practice for Development
of ASCEM Requirements

October 26, 2010

ASCEM-PM-10-05

ASCEM

United States Department of Energy

E_M *Environmental Management*
safety ❖ performance ❖ cleanup ❖ closure

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Printed in the United States of America

Prepared for
U.S. Department of Energy

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_____   10/28/2010
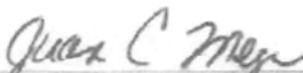Mark Freshley, Pacific Northwest National Laboratory   Date
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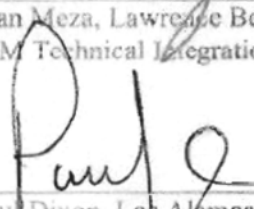

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TABLE OF CONTENTS

LIST OF TABLES AND FIGURES

LIST OF ABBREVIATIONS

ASCEM	Advanced Simulation Capability for Environmental Management
CBP	Cementitious Barriers Partnership
D&D	Decontamination and Decommissioning
DQO	Data Quality Objective
DOE EM	Department of Energy Environmental Management
EPA	Environmental Protection Agency
FY	Fiscal Year
GIS	Geographic Information System
HPC	High Performance Computing
INL	Idaho National Laboratory
LFRG	Low-Level Waste Disposal Facility Federal Review Group
NAS	National Academy of Sciences
NRC	National Research Council
ORR	Oak Ridge Reservation
PA CoP	Performance Assessment Community of Practice
SBR	DOE Office of Science Subsurface Biogeochemical Research
SRS	Savannah River Site

0.0 EXECUTIVE SUMMARY

The Advanced Simulation Capability for Environmental Management (ASCEM) project is developing a state-of-the-art scientific tool and approach for understanding and predicting contaminant fate and transport in natural and engineered systems. This modular and open-source high-performance computing (HPC) tool will facilitate integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for EM cleanup and closure activities. ASCEM is organized into three major thrust areas: Multi-Process High Performance Computing Simulator (HPC Simulator), Platform and Integrated Toolsets (Platform), and Site Applications.

End user involvement is an important aspect of the ASCEM initiative. End users include performance assessment (PA) and risk assessment practitioners, decision-makers, oversight personnel, and regulators who are engaged in the Department of Energy (DOE) cleanup mission. Solicitation of end-user feedback is critical during the initial ASCEM development to ensure that user needs are incorporated into the framework. Subsequent and consistent engagement is key to developing user acceptance and eventual application of the ASCEM toolsets at DOE sites.

Recognizing the importance of end-user involvement, the Site Applications Thrust includes a "user needs interface" task. This task focuses on establishing contact with various end users, soliciting their input about ASCEM development plans, and conveying the feedback to members of the HPC and Platform Thrust areas responsible for tool and code development. Over the long term, the Site Applications Thrust includes several tasks designed to engage and support end users, including site demonstrations, development of protocols, documentation and work flows, and training and support in the use of ASCEM tools.

This report, which represents the first product of the "user needs interface" task, summarizes interactions with a variety of users and synthesizes their feedback into suggestions for development of requirements for the HPC and Platform Thrust areas. It also provides suggestions for potential test cases and demonstrations for use in future Site Applications activities.

Input was obtained through five different activities:

1) <u>Solicitation of comments on the ASCEM proposal</u> – Received thirteen sets of comments from members of the Low-Level Waste Disposal Facility Federal Review Group (LFRG), practitioners, oversight personnel, and other DOE offices.

2) <u>Interviews with potential users at DOE sites</u> – Conducted eighteen different interviews with representatives from a variety of different perspectives at key DOE sites.

3) <u>Discussions with DOE Office of Science Subsurface Biogeochemical Research (SBR) Program participants</u> - The SBR Principal Investigator Meeting included a session to address modeling needs.

4) <u>Participation in a Performance Assessment Community of Practice (PA CoP) Technical Exchange</u> - Through this technical exchange targeted at ASCEM, a broad cross-section of potential users provided feedback.

5) <u>Reviews of Current Performance Assessment Practices</u> - Reviewed documentation from recent performance assessments conducted at DOE sites to develop perspective regarding current practices.

In addition to providing many detailed and constructive suggestions, these discussions allowed ASCEM team members to explain to users the project's goals, objectives, and plans.

During the course of these discussions, the following common suggestions arose:

- Current regulatory modeling approaches have been adequate, but improved capabilities are needed to address future challenges.

- Modeling needs to be integrated with field sampling, demonstrations, monitoring, etc., for a holistic approach to decision-making.

- Structured documentation, transparency of assumptions, and ease of use are important for gaining broad acceptance.

- A graded and iterative approach is critical, including a continuum of modeling complexity from screening to detailed process models.

- Improved capabilities for source-term models (e.g., barrier and waste form degradation and reactive transport for release processes) will help with key challenges.

- HPC needs to be leveraged for better efficiency of uncertainty analyses and process modeling for complex systems.

- End users and decision makers need to be involved in the development process, especially in the Platform Thrust and demonstrations and testing.

- Processes related to surface exposure pathways need to be addressed (e.g., intrusion scenarios, biotic transport, etc.).

Actively seeking end user input has proven invaluable in introducing ASCEM to the user community and helping the ASCEM team to understand user needs. The reviews, interviews and discussions summarized in this document are organized roughly in line with the ASCEM activities in order to facilitate their consideration by ASCEM thrust and task leads.

In addition, this outreach also provided a number of general suggestions, as well as suggestions for a number of potential test or demonstration problems that will be considered during selection of demonstration sites for the Site Applications Thrust area.

1.0 INTRODUCTION

The mission of DOE's Office of Environmental Management (EM) is to complete the safe cleanup of the environmental legacy from the nation's five decades of nuclear weapons development and production, as well as nuclear energy research. The EM mission represents one of the most technically challenging and complex undertakings in the world—one that requires investment in remediation science and technology development.

Advanced simulation capabilities will play an important role in improving the risk and performance assessments necessary to guide and defend future cleanup decisions. Two objectives will guide development of these capabilities:

1) Advancing the state of the science with improved technical understanding and modeling capabilities

2) Recognizing the practical, application-specific needs associated with regulatory analyses that support decision-making.

These objectives are, in fact, complementary. Sound decision-making requires sufficient technical underpinning (need to advance the state of the science), but also requires efficient approaches that enable timely and cost-effective decision-making (practical, application-specific needs). Recommendations related to these two types of needs are identified below.

1.1 Scientific Needs

In response to direction from Congress, DOE-EM developed the *Engineering and Technology Roadmap* (Roadmap) identifying technology gaps in the EM program and strategies to address them [1]. In response to a request for assistance from EM, the National Research Council (NRC) of the National Academy of Sciences (NAS) provided *Advice on the Department of Energy's Cleanup Technology Roadmap: Gaps and Bridges*. That NRC report identifies and ranks the principal science and technology gaps that could adversely affect EM's ability to meet its cleanup milestones on time and/or on budget and provides recommendations for improving the Roadmap [2]. *Table 1.1* shows the principal Roadmap gaps and their NRC priorities for the DOE Groundwater and Soil Remediation Program.

Table 1.1 Principal Groundwater & Soil Remediation Science and Technology Gaps and their Research and Development Priorities.

Number	Gap	Priority
GS-1	Contaminant behavior in the subsurface is poorly understood.	High
GS-2	Site and contaminant source characteristics may limit the usefulness of baseline subsurface remediation technologies.	Medium
GS-3	Long-term performance of trench caps, liners, and reactive barriers cannot be assessed with current knowledge.	Medium
GS-4	Long-term ability of cementitious materials to isolate wastes is not demonstrated.	High

To address these gaps, NRC provided a series of recommendations, one of which focused on the development and use of advanced computational models. NRC advised that these modeling tools should:

- Incorporate understanding of site geohydrology and contaminant geochemistry, with the goal of improving the currently insufficient scientific knowledge base (GS-1)

- Include robust models of caps/covers, barriers, and cementitious materials/ waste forms (GS-3)

- Incorporate appropriate uncertainty (GS-1, GS-2, GS-3, and GS-4)

- Account for natural and anthropogenic spatial and temporal changes, together with field data to calibrate these models (GS-3 and GS-4)

- Develop predictive capabilities to understand contaminant behavior and to support developing and implementing effective and sustainable remediation approaches (needs previously indentified in internal workshops and reviews [3, 4, 5]).

1.2 Regulatory Application Needs

Practical application of performance and risk assessment models place a premium on higher-level considerations, such as:

- Ability to apply varying levels of complexity

- Optimizing expenditures and effort on data collection, including improved methods for parameter estimation

- Using more complex models and data to provide the technical underpinning to support key assumptions and reduce conservatism in key areas

- Effectively explaining uncertainties in model results and supporting decision-making

- Clear documentation with transparency and defensibility of assumptions

- Using models as part of an integrated approach to support decision-making.

The key concept of a graded and iterative modeling approach has evolved consistent with NAS recommendations regarding scientific and regulatory applications of ground water models [6] and multiple agency recommendations (e.g., US Environmental Protection Agency [7], International Atomic Energy Agency [IAEA] [8], US Nuclear Regulatory Commission [9], National Council on Radiation Protection and Measurements [10]). The graded and iterative approach is favorable because performance and risk assessments may involve hundreds of contaminants, exposure pathways/scenarios, features, events, and processes, many of which will be inconsequential to cleanup decision-making. It is neither practical nor necessary to collect all of the data and defend all of the assumptions surrounding data points that are inconsequential to the task at hand (e.g., the EPA Data Quality Objectives [DQO] process [11]).

A graded and iterative approach provides a defensible means to eliminate the inconsequential aspects of a problem from further consideration through 1) screening approaches, and 2) incrementally increasing complexity for the aspects with greatest influence on the pending decision. Decision support tools are critical for this approach, which requires, in each iteration, prioritization of areas in which to add complexity and collect additional data. Each iteration also requires evaluation of design or remedial action options. Within this construct, it is possible to continue to use a less complex model in subsequent iterations, with a more complex model underlying it and providing technical underpinnings, thus reducing conservatism in the overall regulatory model.

1.3 Advanced Simulation Capability for Environmental Management

In response to the NAS and internal review recommendations, DOE-EM launched the Advanced Simulation Capability for Environmental Management (ASCEM) initiative to address the key challenge areas in *Table 1.1*. ASCEM is developing a state-of-the-art scientific tool and approach for understanding and predicting contaminant fate and transport in natural and engineered systems. The modular and open-source HPC tool will facilitate integrated approaches to modeling and site characterization that enable robust

and standardized assessments of performance and risk for EM cleanup and closure activities. In addition, the integrated model will address broader application-oriented needs, such as incorporating capabilities for predicting releases from various waste forms, identifying exposure pathways and performing dose/risk calculations, systematic uncertainty quantification, and decision-making during the end of the assessment process. The capabilities will be demonstrated at selected sites and then applied to support the next generation of performance and risk assessments across the DOE-EM complex.

As depicted in *Figure 1.1.*, ASCEM is organized into three major thrust areas: Multi-Process High Performance Computing Simulator (HPC Simulator), Platform and Integrated Toolsets (Platform), and Site Applications. The HPC Simulator Thrust includes tools supporting the modular simulation capability for barrier and waste form degradation, multiphase flow, and reactive transport. The Platform Thrust includes tools to facilitate model development and execution, parameter estimation, uncertainty quantification, decision support, and risk analysis. The Site Applications Thrust includes activities designed to identify demonstration problems for the ASCEM tools and actively involve the user community in toolset development.
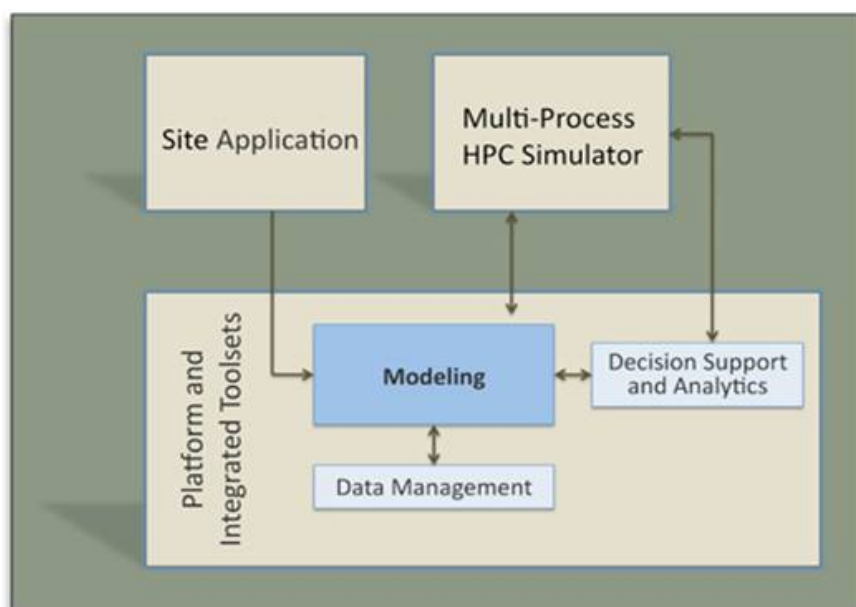
Figure 1.1 ASCEM Project Structure

End user involvement is an important ASCEM component. End users include performance assessment and risk assessment practitioners, decision makers, oversight personnel, and regulators who are involved in the DOE-EM cleanup mission. Solicitation of end-user feedback is critical at the early stages of development to ensure high priority user needs are incorporated into the framework. Engagement of end users throughout ASCEM development is expected to facilitate the adoption of ASCEM tools for practical application at DOE sites.

Recognizing the importance of involving end users, the Site Applications Thrust includes a "user needs interface" task to establish contact with end users, solicit their input about ASCEM development plans, and convey the feedback to appropriate members of the HPC Simulator and Platform Thrust areas. Over the longer term, the Site Applications Thrust includes several additional tasks designed to engage and support end users, including site demonstrations, development of protocols, documentation and work flows, as well as training and support in the use of the resulting capabilities.

1.4 Purpose of this Report

The user interface task in the Site Applications Thrust was conceived to solicit input from a diverse cross-section of the DOE end-user community (see Section 2 for details). This report, which represents the first product of this task, summarizes the results of interactions with a variety of users and synthesizes their feedback into suggestions for development of requirements for the HPC Simulator and Platform Thrust areas. It also includes suggestions for potential test cases and demonstrations that could be used in future Site Applications activities. Consistent with the nature of tasks in the Platform and HPC Simulator Thrust areas, two levels of information were obtained:

1. Higher-level implementation-related information supporting key tasks in the Platform Thrust (e.g., regulatory and programmatic considerations, implementation of a graded and iterative approach, and user interface suggestions)

2. More detailed technical information supporting conceptual model- and data-related tasks in the Platform Thrust and identification of modeling needs for the HPC Simulator Thrust (e.g., environmental conditions found at different sites, engineered features being used, data availability, conceptual models and modeling approaches, and specific processes needing consideration).

Emphasis was also placed on the following:

- Identifying key areas where improvements would be most beneficial (e.g., where simplifying assumptions consistently result in overly conservative approaches and improvements in implementation efficiency)

- Identifying available data sets and potential demonstration problems to be considered for site demonstrations or individual toolset test or validation cases.

2.0 PROCESSES FOR OBTAINING USER INPUT

End user input was obtained through five different activities:

- **Comments on the ASCEM proposal** - The fiscal year (FY) 2009 ASCEM proposal was submitted to a variety of DOE organizations and distributed to LFRG for review and comment. LFRG and DOE Field and Headquarters personnel provided thirteen sets of comments. The comments were considered during the development of the ASCEM implementation plan and are also reflected in this report.

- **Discussions with DOE Office of Science Subsurface Biogeochemical Research (SBR) Program participants** - SBR conducted its principal investigator meeting in March of 2010. The meeting included a breakout session on "Modeling and Simulation of Subsurface Systems," which was designed to address a series of issues:

  - Identifying the weakest links in reactive transport models in terms of processes or parameters limiting their predictive ability

  - Discussing the modeling role in experimental design and interpretation

  - Identifying new theories for HPC model development and application

  - Discussing the importance of computer science and applied mathematics for model improvements

  - Incorporating new kinds of characterization and other data into models to improve predictive abilities

  - Optimizing the relationship between required data and increasing levels of complexity, recognizing that future models will be data limited.

  Examples of observations from the breakout session include:

  - Modeling works best as part of an integrated project using a holistic approach.

  - Modeling should be done with the least amount of complexity defensibly possible, but a balance is needed between overkill and oversimplification.

  - Detailed modeling can be used to evaluate the relative importance of complex processes.

– Weak links for modeling applications typically include information on source terms and representation of geochemistry (e.g., sorption data, distribution coefficients in most cases).

– In spite of over twenty years effort, the task of building thermodynamic databases used to support reactive transport models has not been completed. However, good progress has been made

– At some sites, uncertainty analysis and reactive transport modeling is reviewed and approved by regulators, and at other sites, less sophisticated models are used for the regulatory interface.

– Key challenges include colloid-facilitated transport, dissolved organic matter and microbial reactions, coupled models, and computational requirements for representing even simple complexation reactions.

- **Participation in a PA CoP Technical Exchange** - The PA CoP Technical Exchange provided a venue for performance and risk assessment practitioners, decision makers, and regulators to share experiences with both ASCEM and Cementitious Barriers Partnership (CBP) developers. Additionally, detailed discussions occurred regarding the integration of ASCEM and CBP. The agenda, list of participants, video files and presentations are available on the Technical Exchange website (http://srnl.doe.gov/copexchange).

Suggestions were consistent with initial LFRG comments on the ASCEM proposal, and those from interviews with DOE site users. The following suggestions were consistent discussion topics and reflect the primary focus of the broader feedback received from users to date:

– Address prospective challenges - Although existing regulatory modeling approaches have been adequate to date, greater cleanup challenges await, and ASCEM and the CBP should advance process modeling capabilities to help optimize future decision-making.

– Take an integrated approach - ASCEM and CBP modeling should effectively integrate with field activities (e.g., sampling, demonstration, characterization, monitoring) to enhance modeling capabilities and support decision-making.

– Provide compatibility and ease of use - The Platform needs to facilitate structured development of documentation, transparency of data and assumptions, and ease of use for a range of potential users from a regulator/reviewer perspective; compatibility with currently accepted regulatory models, as needed, would also be a benefit.

– <u>Provide for a range of complexity</u> - Implementation of a graded and iterative approach that includes flexibility for a continuum of modeling complexity (from screening models to detailed process representations) will be critical (also within a single assessment for composite analysis).

– <u>Improve source term capabilities</u> - Improved capabilities for source-term models (e.g., barrier and waste form degradation and reactive transport for release processes) will help with key challenges.

– <u>Exploit computing advances</u> - Leverage HPC capabilities to improve the efficiency of uncertainty analysis, utilize increased grid resolution, address reactive transport, and use increased model dimensionality for complex problems.

– <u>Involve users and decision makers</u> – Seek opportunities for active involvement of users and decision makers in the development process, including design of Platform (especially decision toolsets), testing of modeling tools, and potentially using individual modules to demonstrate benefits for shorter term needs (e.g., supporting PA analyses).

– <u>Address exposure assessment</u> – Although initial efforts may focus on fate and transport aspects, ASCEM will eventually need to address the variety of processes associated with exposure analysis, including surface processes.

- **Interviews with potential users at DOE Sites** - Eighteen separate interviews were conducted with National Laboratory, site contractor, and/or DOE Staff at Los Alamos, Idaho, Savannah River, Lawrence Berkeley, Pacific Northwest, Lawrence Livermore, and Oak Ridge National Laboratories, as well as the Hanford site and Portsmouth/Paducah. The interviews ranged from detailed one-on-one or small group discussions to larger group discussions involving a mixture of DOE, contractor, and National Laboratory personnel. Future plans include considering the need to update this document to include sites missing from the initial interviews. These interviews were the primary source of information for this report.

  The set of questions developed to guide the interviews and provide a common framework for discussion is provided in Appendix A. Each interview took one to two hours and involved open discussions of ASCEM and end user expectations. Generally, site personnel reacted positively to the interview process. They agreed that the interviews facilitated greater understanding of ASCEM goals. The interviews are the primary basis for the information provided in Sections 3-5. (Raw information from the site interviews and reviews has been summarized into the tables provided in Appendix B.)

- **Survey of current approaches for performance assessments (see Section 6)** - As part of its planning process, ASCEM conducted a review of codes and data

used in recent performance assessments and composite analyses prepared in accordance with DOE Order 435.1 requirements. In general, performance assessment analyses are required to support radioactive waste disposal actions, while risk assessments are conducted to support remediation decisions (although there can be some overlap depending on the regulations governing a given disposal facility). The review was designed to identify the codes, methodologies, main assumptions, and key data sets used in these analyses. The review was conducted for several major DOE-EM sites and is summarized in Section 6.

3.0 GENERAL SUGGESTIONS FROM USERS

A number of suggestions from the user interactions applied to the project in general. These needs and suggestions draw attention to higher-level practical and philosophical concepts directed at making the ASCEM toolsets more attractive to the end-user community. The suggestions are briefly summarized below.

- **Models provide input for regulatory decision-making** - Higher-level representatives of the user community emphasized the importance of modeling's role in the regulatory decision-making process. Decision-makers must explain to a broad, often non-technical audience how results contribute to a decision. Effective tools for visualization and uncertainty quantification, including sensitivity or importance analysis, play a significant role in interactions with such stakeholders. Transparency and documentation of both assumptions and the modeling process are also critical (see Section 3.4).

- **Graded and iterative approach for efficient application of models** – Users noted that current implementations of regulatory calculations often involve time constraints that place a premium on the efficient use of resources. Therefore, users emphasized the need to develop a toolset that can efficiently solve problems, or specific aspects of problems, with relatively simple models or data. The toolsets must also have the ability to iteratively increase complexity for the most challenging aspects of a problem in the context of the decision to be made.

  The use of such a graded and iterative approach for regulatory modeling is common throughout the DOE complex and recommended by other organizations, including the Environmental Protection Agency [7], the International Atomic Energy Agency [8], and the Nuclear Regulatory Commission [9]. While improving process efficiency, this approach also delivers a methodology for prioritizing and providing objective justification for collecting additional information required to support more complex models for areas of particular concern. The most complex models should be focused on the most important aspects of the problem.

  A number of end users commented that computational limitations were a significant contributor to the need for simplifying assumptions and modified

approaches. To minimize such limitations, ASCEM's graded and iterative approach will incorporate the most recent advances in HPC.

- **Integrated use of models with field, laboratory and other inputs** - It is important to develop a toolset that can utilize an integrated approach to decision-making. An integrated approach considers information obtained from activities in the field and laboratory, interactions with stakeholders, and monitoring in addition to the results of modeling efforts. It does not overemphasize any one activity as the key to decision-making and recognizes that different information (models, data, etc.) may be the driver depending on the problem at hand. This is consistent with the NAS view that models are only one part of an integrated approach to providing a basis for decision-making [6].

- **Regulator needs for accessibility, documentation and transparency of assumptions** - User feedback indicated an increasing desire for regulators to either independently conduct modeling (in the case of organizations with modeling expertise), or to independently run simulations using a contractor model to explore sensitivities and gain a better understanding of the analysis. This implies ASCEM tools should be accessible for confirmatory simulations or what-if sensitivity analyses by those with a basic level proficiency. While it is important to recognize that application of any model requires a given level of proficiency and training, the ASCEM toolsets will be accessible to those without specialized computational or code development expertise.

  In simulations of subsurface flow and transport, assumptions are required for generating many of the model parameters. Regulators and reviewers expect clear documentation and transparency of the assumptions made. Documentation and traceability of the modeling process is an important component of regulatory analyses. Regulators also expect explanations of the key assumptions that most influence decision-making, which highlights the importance of effective uncertainty and sensitivity analysis tools.

- **Learn from development of other successful regulatory codes** - The ASCEM team should leverage development and implementation approaches used for widely accepted computer codes such as, GoldSim [12], the MODFLOW/GMS family of codes [13] and the RESRAD family of codes [14]. These codes enjoy widespread acceptance because developers actively worked with the regulator and user communities. Other computer codes, such as FEHM, TOUGH, STOMP, PFLOTRAN, and PORFLOW, gained user acceptance through specialized applications (flexible meshing, decay chains, etc.) designed to solve user-identified problems. Several of these codes have been accepted for regulatory analyses at DOE-EM sites.

- **Plan for network, access, and computer security protocols at different DOE sites -** Firewall and security protocols often restrict computing at DOE sites. The

ASCEM toolset will need to accommodate these security restrictions as well as users' need to remotely access HPC computers, databases, or other files. Thus, developing a toolset that operates smoothly across the DOE Complex will be a challenge. When intense efforts are associated with executing production runs in advance of regulatory milestones, competition for time on HPC resources could also become a concern.

4.0 SUMMARY OF USER INPUT FOR PLATFORM AND INTEGRATED TOOLSET THRUST

Developing models for understanding and predicting contaminant fate and transport in natural and engineered subsurface systems requires the collection, management, and analysis of large and diverse data sets, and a thorough understanding of modeling and simulation tools. To meet these requirements, the Platform will provide the following:

- A user interface environment that facilitates the complex process of conceptual model development and code application to a given site and problem

- A set of tools incorporated into a consistent framework that permits a modeling approach that is flexible, maintains quality assurance (QA) standards and data integrity, and increases user efficiency

- Capabilities for advanced information and data management, parameter identification, uncertainty quantification, decision support, risk assessment, and visualization

- Seamless interfacing with the new ASCEM HPC simulator as well as some commercial and open source modeling tools involved in pre- and post-processing for the HPC models.

For most users, the Platform will be the most visible aspect of ASCEM. It therefore elicited the greatest number of suggestions. User suggestions have been divided into several categories, roughly aligned with ASCEM work areas.

4.1 Task Level User Input – Platform Thrust

- **Data Management -** Effectively managing the staging and movement of data, and ensuring its availability.

  - Ability to link with existing databases - Users identified a number of different databases in a variety of different forms with different access provisions, integrated across different sites, and with different levels of effectiveness. A further effort to gather detailed information on DOE-EM databases was

recommended. Users suggested leveraging available database structures whenever possible. Specific examples of databases identified during the interviews are provided in the data management table in Appendix B.

– <u>Managing model data input and error checking</u> - Users indicated that a common challenge with assessments involving multiple data structures, models, and tools is the transfer of information from one model or tool to another. These transfers are a common source of errors in performance and risk assessment modeling. In a probabilistic framework, there is also the added challenge of tracking changes to a parameter in one model or component that needs to be reflected in a similar or dependent parameter used in another model or component for each realization. Capabilities to automate and make the links between models and tools more transparent would be a significant benefit. Users identified a number of other areas of interest, including managing local data versus global data (e.g., thermodynamic databases), and addressing challenges involved in translating local data in different formats for use in model applications.

– <u>Integration of data from multiple sources and database maintenance</u> – Users identified a variety of integration issues, reflecting the multiple types of data that will need to be maintained. The data must also be used for parameter estimation and, ideally, for consideration in the development of direct linkages between models and databases. The linkage of borehole logs, analytical data, etc., with spatial data management systems (e.g., Geographic Information System [GIS]) was identified as a key need. Also key were data review and format tools for easier interoperability between databases and models, and tools to optimize the value of existing data for parameter estimation and process description—data that may be of different quality levels and may exist in multiple locations. Users also identified the need to address access and firewall considerations at most DOE sites. One user community suggested that the Yucca Mountain Project database be an end member-type example for database maintenance and usability.

– <u>Traceability and transparency, data tracking, and provenance</u> – From a review or regulator perspective, the need for traceability and transparency of assumptions and input data is critical (Section 3.4). Data tracking and provenance information need to be maintained and accessible to support internal and external reviews of modeling work, as well as any calculations that depend on that information. Regulators and reviewers expect transparent documentation of key assumptions regarding data and conceptual models that impact conclusions. Users suggested that while the interface should be designed for modelers, there should be capabilities for reviewers to identify key assumptions and access supporting information.

- Capability to produce information in formats that support known reporting requirements - Some users identified the benefits of developing databases and queries/reports with an eye towards specific reporting requirements in different regulatory frameworks. For example, if a site-wide monitoring report requires information in a specific format, the Platform should be able to produce an appropriately formatted query and report. Users also requested the capability to compare analytical data with model results as part of compliance with DOE Order 435.1. It may also be possible to develop standard formats for use across the DOE-EM complex. Archiving information that will eventually be passed on to other organizations, such as Legacy Management, also needs consideration.

- Support for different levels of access for site users, regulators, and the public - While the need for different levels of access was not consistently mentioned across the DOE sites, there were cases in which regulators or the public required access to data. To facilitate this, the ability to provide levels of access for different types of information would be helpful.

- **Core Platform, Model Setup and Analysis** - Providing user access to ASCEM functions via graphical interface, tools for automated job launching and monitoring, and providing a set of Application Programmer Interfaces for constructing and integrating ASCEM toolsets.

  - Accommodate multiple levels of complexity- Users placed great emphasis on the need for a defensible means of eliminating inconsequential aspects from further consideration in remediation decisions. They want the ability to start with simplified screening approaches and incrementally increase complexity for aspects with the greatest influence. However, they noted that when applying the graded approach, it is important not to oversimplify such that the influence of an important process is missed.

    Users suggest that the platform first apply simplified tools to conduct initial screening to reduce a problem to a manageable size. The Platform should then provide decision tools and coordinating functions to incrementally identify the aspects requiring increased complexity. In this efficient approach, the most complex modeling and associated data requirements are only conducted when necessary for decision support. Users also highlighted the benefits of using two or more different levels of detail (or modeling approaches) for the same problem for reality checks. Integration of modeling with field activities also helps to improve confidence by providing an objective point of comparison.

  - Traceable record of each assessment (models and versions used, inputs, etc.) - Users emphasized the importance of having a traceable and reproducible record of all the computer codes and versions, input and output files, and data sources used for a given assessment. For reviewers and regulators, a file that included

direct links to the input files, data sources, etc., would also be useful. Users suggested that the tools include the capability to identify changes between different simulations in cases where multiple, separate calculations (sensitivity or uncertainty analyses) are conducted.

– Represent multiple sources of contamination at multiple scales and complexity - Site-wide assessments and composite analyses involve calculations covering large areas and potentially involving hundreds of different sources. The sources at any given site can range from lightly contaminated concrete slabs, to tank farms with multiple tanks containing high-level waste. Users would like models of varying complexity to represent individual sources, commensurate with the level of concern. Subsequently, these more complex "near-field" models must be integrated into large-scale, site-wide models. (Appendix B contains a number of the specific process and conceptual model considerations identified).

– Interoperability of models and tools - Current modeling approaches often depend on multiple models and tools which are not interoperable. Users identified passing and conversion of information between tools as a common source of errors, as well as a source of inefficiency in requiring the checking and rechecking of information. Similarly, as deterministic and probabilistic approaches are implemented, models need to "play well together." Users requested the capability to automatically propagate changes in parameter values, distributions, or assumptions in one module to match similar or dependent parameters and assumptions in others. Examples of data that may need to be consistently applied included: saturation profiles; porosity; contaminant concentration; lithology; permeability; and geochemical parameters.

– Recognize regulator interests - At many DOE-EM sites, regulators participate in conceptual model and scenario development as assessments are being conducted. The Platform should support such processes. For example, it would be useful to have a means to evaluate available data relative to both Data Quality Objectives and options for conceptual models in order to identify data gaps. During their review of analysis results, regulators generally require a demonstration of understanding of the system being modeled. Users also requested recognition that regulators show bias towards less complex models that are easily explained, and may require abstractions from more complex models or technical underpinnings using more complex models.

An important part of demonstrating understanding is the ability to identify key assumptions that may have the greatest impact on decision-making. Thus, the Platform should summarize key assumptions in a manner that allows external reviewers to explore them in varying levels of detail. Regulatory agency staff expressed the desire to conduct or access what-if type calculations in order to

explore the impacts of specific changes to existing models. They also sought the ability to clearly distinguish the benefits of different remedial or design options. Visualization and effective presentation of the basis for specific decisions were also deemed important when working with regulators and stakeholders (see those specific discussions in Sections 4.4 and 4.5).

– <u>Availability of specific tools for practical applications</u> - Users identified several areas in which the Platform could develop specific tools to address specific needs. Development of disposal facility waste acceptance criteria generally involves back-calculation of allowable concentrations of each contaminant that results in dose or risk at the allowable limit. Additionally, there is often a need to develop different limits for a given contaminant depending on the type of waste form or container holding it. Another approach is to develop a model that executes quickly and can assess the suitability of a specific waste container.

The Nuclear Regulatory Commission uses "barrier analysis" to assess the effectiveness and importance of different barriers for a specific problem. In a barrier analysis, different model features are removed to assess the removal's impact on conclusions. Users agreed that such functionality would be useful in the Platform.

In order to demonstrate that a facility is operating within the expected performance envelope, DOE Order 435.1 requires comparison of monitoring results with model projections. Generally, predicted concentrations for a given location (e.g., depth in vadose zone, aquifer) are compared with peak observed concentrations in monitoring wells. In the future, other indicators may be used for comparisons. Users said that automating these comparisons would contribute to improved integration of field observations and modeling efforts.

• **Uncertainty Quantification -** Managing the development of input distributions and calculations necessary to quantify the uncertainty in the results of an assessment based on variability and broader uncertainties associated with the inputs.

– <u>More efficient or improved computing approaches for uncertainty quantification</u> - Users regularly identified efficient computing approaches for uncertainty quantification as a major need. Users mentioned computational limits necessitating a high reliance on 1-D abstracted models when trying to implement hundreds of time-consuming realizations with more complex models. Users wish to take advantage of increased computing power to develop alternative methods to enable full probabilistic uncertainty analyses with more complex models.

- Need for a catalog of methods for uncertainty quantification with guidance - Many of the comments in DOE-EM reviews of deterministic and probabilistic assessments concerned the development of input distributions and the implementation of uncertainty analyses. Users expressed a desire for a "decision tree" for guidance in choosing the most appropriate uncertainty analysis method. They requested that this "decision tree" include development of input distributions, experimental/measurements/design uncertainty assessment, modeling uncertainty, conceptual model and scenario uncertainty, and risk assessment. Tools to facilitate input distribution development were also a particular need.

- Tools to help decision-makers explain uncertainties - With a decision-maker's needs in mind, users emphasized the importance of uncertainty quantification tools in the Platform. Approaches for illustrating/presenting results of uncertainty analyses and sensitivity (importance) analyses in layman's terms were also emphasized. These would answer the decision-makers' need to identify the most significant contributors to uncertainty throughout the assessment process and present those concepts to different audiences.

  Decision-makers also need to distinguish the effects of features and assumptions related to future scenarios from the effects of variability in sensitive model parameters (see "Aleatory and epistemic uncertainties and assessing total uncertainty" below). They must distinguish sensitive parameters that significantly impact conclusions from those that may alter predicted doses but leave conclusions unchanged.

  Uncertainty quantification can also improve comparisons between monitoring results or field data and models. Currently, peak monitoring results are often compared with model predictions. Single point peaks can exceed the model predictions at an individual well, but generally not over a significant area. Better approaches will allow these comparisons to recognize the uncertainties in field measurements and model results.

- Aleatory and epistemic uncertainties and assessing total uncertainty - Assessments typically involve two general categories of uncertainty: aleatory (variability) and epistemic (structural). Users emphasized the need to account for both categories and reflect their relative importance in the context of a particular problem. Identifying reducible aleatory uncertainties, which are due to inherent variability associated with the natural environment, will facilitate implementation of appropriate site characterization, monitoring methods, or field demonstrations as well as the selection of appropriate conceptual and numerical models. It is also beneficial to quantify the influence of epistemic uncertainties associated with a lack of knowledge (e.g., choice of conceptual models or future evolution scenarios for specific features, events, or processes).

The uncertainty tools should identify the relative importance of, and uncertainties associated with, different barriers (e.g., waste form, container, vault or tank, vadose zone, etc.) in terms of the projected dose. As mentioned, the Nuclear Regulatory Commission uses the term "barrier analysis" to indicate such a quantitative estimate of 1) the influence of different barriers, and 2) assumptions regarding failure scenarios, different facility designs, or remediation technologies.

– Isolate significance of uncertainties that change in time and space - Uncertainties and the importance of different parameters are often a function of time and space. For example, if peak doses result from H-3, one set of parameters will control uncertainties, which will generally occur early in time. However, if the peak doses result from U-238 + progeny, the uncertainties will likely be associated with other parameters and occur later in time. Because specific contributors to dose must be isolated, there is a need to separate parameters that are important for early peaks from those that impact later peaks (due to different radionuclides).

Similarly, for situations with multiple source terms that discharge to different receptor locations, users need to quantify uncertainty and importance as a function of the location of dose. Tank PAs have shown that important parameters for a dose at one location from a specific tank are different from the important parameters for a peak dose at another location from a different tank. General uncertainty and sensitivity analysis may not be able to separate such spatially- and temporally-driven needs.

– Consistent updating of similar or dependent variables in multiple models – When using Monte Carlo simulations for uncertainty analyses, errors can occur when a variable changes in one model or component for a given realization, but similar or dependent variables are not updated in others. Users sought approaches to identify and track similar and/or dependent variables in multiple modules/models in order to update all of them in individual realizations of an analysis.

– Approaches for effective abstraction - Users would like the ability to continue using abstraction or simplified representations in risk and performance assessments—especially to support probabilistic models. Therefore, they need defensible abstraction approaches that use more complex models and/or field or laboratory data for technical underpinning.

• **Decision Tools** – Supporting decision-making for site application users, modelers, project managers, stakeholders, and decision- and policy-makers.

– Decision support for graded and iterative approach - Users highlighted the role of decision tools to support the graded and iterative approach for assessments.

Iterative assessments require robust mechanisms for identifying and prioritizing areas that require detailed consideration. Decision support tools interpret results from increasingly complex models to prioritize areas where additional analytical detail can reduce key uncertainties or support key assumptions. Some consideration of cost-benefit would also assist with prioritization. The ability to abstract results from complex models for use in decision-making tools was also identified as a potential benefit.

In order to compare how assumptions can affect conclusions, users requested the ability to conduct parallel modeling efforts using different conceptual models, or different levels of complexity for specific processes or barriers. This capability could also support decisions around increasing complexity. When iteratively coupled with model testing, evaluating multiple conceptual models would also help in determining data needs. These ideas are connected to the concept of barrier analysis, which can identify and quantify the relative impacts of different barrier designs and failure scenarios on overall performance.

– Integration and optimization of modeling, monitoring, and data collection - Decision tools are needed for improved integration and optimization of modeling, monitoring, and data collection activities. Integrated approaches that combine these activities are expected to improve decision-making, result in more efficient use of resources, and reduce undue reliance on any single activity. In combination with modeling, approaches that optimize the use of field data, monitoring, and process understanding can limit the need to collect large amounts of field data that may not significantly impact decision-making.

Users noted that integrated decision tools can determine the optimum type and placement of sensors and monitoring points based on existing field information and model results. Decision tools can also optimize the appropriate frequency of sampling events, analyses, and number of samples. Through interim assessments and modeling results, this information can reveal situations appropriate for remediation technologies or design changes.

– Support for DQO process - Users suggest that functionality to implement the DQO process will be useful in identifying data gaps, and in dealing with the many explicit decisions made during the modeling process. The DQO Process is a seven step, iterative planning approach for environmental data collection activities [11]. It provides a systematic approach for defining the criteria for a data collection design, including: when, where, and how to collect samples or measurements; determination of tolerable decision error rates; and the number of samples or measurements that should be collected.

– Systems approach for cost/benefit analysis and evaluation of remedial options - Users recommended implementing systems risk analysis tools to support

decisions concerning D&D, remediation, and technical project risks. Using GIS or other spatial mapping tools, a systems analysis approach can document and rank according to risk the bounds of known and suspected contaminated media and potential high-risk transport pathways. Users can employ this information to identify areas that would benefit from further site characterization. Information gained from the systems approach would also increase understanding and contribute to the development of cost-effective remediation decisions. A formal systems approach can also assist the regulatory process for treatability tests, feasibility studies, and selection of remediation options.

- **Risk Assessment -** Providing a comprehensive risk resource enabling the flexibility/adaptability to support all regulatory environments as well as synthesize risk with other primary data/information components in support of data collection and decision-making processes.

  – <u>Multiple regulatory environments with different approaches</u> - The risk assessment toolset needs to provide data, tools, and guidance to enhance the integration of ecological and human health risks into the EM decision-making process. The toolset needs to provide access to DOE and other regulatory guidance, standard risk and dose parameters, uptake and concentration ratio data, and dose and risk calculation tools for human and ecological exposures. The risk assessment toolset should also utilize currently approved risk and dose methodologies, models, dose factors, and toxicity values from different regulators (e.g., USEPA, Nuclear Regulatory Commission, DOE), as well as provide the capability to integrate the latest research in these areas.

  – <u>Processes associated with surface exposures</u> - In addition to the standard exposure scenarios (drinking water, irrigation, etc.) associated with the groundwater pathway, users have identified the need to address the following: surface exposure associated with inadvertent intrusion scenarios; erosion of covers; transport and exposure via flora and fauna that come into direct contact with waste or radionuclides; uptake in plant roots; erosion; resuspension; and dust loading. The number of potential processes is often site-specific and can multiply quickly, thus prioritization will be important.

- **Visualization -** Evaluating different aspects of mathematical and conceptual site models, viewing and analyzing simulation output and derived quantities (e.g., geochemistry, contaminant concentration, and moisture content), and effectively transferring information to decision makers and the general public.

  – <u>Ability to translate a variety of different data formats</u> - Visualization of diverse types of data represents a considerable challenge. Sites use multiple formats for site conceptual models, as well as multiple commercial tools for generating different aspects of those models. If there is no visualization/display tool

available for a particular data format, then either 1) the source data file must be translated for an existing visualization/display tool, or 2) a new reader must be generated for the visualization application.

– Movies and animations - Users emphasized the value of animations to show the evolution of key processes over time (moisture, redox, concentrations, etc.). Movies and animations have proven extremely effective in interactions with stakeholders and regulators. Specific suggestions included allowing users to interactively view the influence of changes in specific inputs, for example using "sliders" (sliding bars associated with varying input values) linked to a graph of an output. In general, users require the ability to plot nodal distributions of key variables, illustrate changes over time, and represent changes in results associated with different assumptions.

– Illustrating uncertainty and sensitivity results – Because the concept of uncertainty is difficult to explain, users requested visualization tools to present uncertainty quantification results in an easily understood format. Also critical is the ability to develop specific plots to support importance analysis for input parameters and assumptions. This will allow the clear identification of problem aspects important to decision-making versus those that are not.

– Error checking and regulator preferences for visualization - Practitioners, reviewers, and regulators need to plot intermediate results (e.g., flux to water table, release from source terms, performance of specific "barriers") as a means to understand system behavior. Intermediate results allow users to confirm that a model is working as expected. They also help with debugging model simulations. Plotting intermediate results also supports "barrier analyses" that quantify the relative importance of different features in the system.

The Nuclear Regulatory Commission requests that derived input distributions be plotted against available data on the same graph. This helps to illustrate the relationship between what is known and what is assumed for a distribution. Visualization tools can also be useful in debugging assignment of material properties in a mesh. Through visualizations, reviewers can quickly show material properties for a specific region. To simplify reviews and error checking, users requested the ability to place the cursor over a specific grid cell or location on a mesh and have the assumed material properties appear onscreen.

5.0 SUMMARY OF USER INPUT ON PROCESSES AND FEATURES FOR HPC THRUST

The toolsets that compose the ASCEM Platform support and streamline the process of creating ensembles of conceptual models to quantify the associated uncertainty,

sensitivity, and risk. These conceptual models span a range of process complexity, potentially coupling hydrological, biogeochemical, and geomechanical processes. The HPC Simulator thrust provides a flexible and extensible computational engine that simulates the coupled processes and flow scenarios described by these conceptual models.

Users provided multiple process modeling needs for consideration during development of the HPC tools. *Table 5.1* identifies the user-identified modeling needs.

Table 5.1 User Suggestions for Process Model Needs

Area of Need	User Suggestion
Multiphase flow and transport	· Include saturated and unsaturated flow and transport of contaminant phases, taking into account ranges of porosity and nonlinear permeability relationships for porous, fractured, and porous-fractured media · Multiphase flow and transport including: LNAPL and DNAPL plumes; density effects; dual (or multiple) continuum approaches; non-isothermal conditions; and colloid transport
Vadose zone/groundwater interactions	· Include ability to simulate flux from vadose zone to groundwater (and from groundwater to the vadose zone), described in terms of being able to review intermediate results (fluxes from source region, vadose zone-groundwater interation) · Include coupled, rather than linked vadose zone-groundwater flux · Transition to solving unsaturated flow or groundwater only when necessary
Groundwater flow and transport	· Include three-dimensional transient groundwater flow and transport, robust water flow and transport model, as well as porous, fractured and porous-fractured media
Reactive transport	· Incorporate geochemical models and modeling solubilities, pH, and redox conditions, equilibrium and non-equilibrium chemistry · Incorporate multicomponent reactive chemistry, and complex reaction networks for small-scale experiments to first-order reactions at the field scale · To help with convergence, code should allow automatic elimination of low-concentration species · Include capability to define new reactions in a modular fashion
Groundwater/surface water interactions	· Include algorithms to allow complex interactions between surface water bodies (streams and rivers), vadose (unsaturated) zone, and groundwater systems, including sediments
Surface water flow and transport	· Both arid and humid sites have a need for surface-water transport, coupled with atmospheric boundary conditions and watershed infiltration, though this may not be an initial emphasis for ASCEM

Table 5.1, continued

Area of Need	User Suggestion
Atmospheric interface	· Include interface of unsaturated zone with atmospheric (boundary) conditions · Include representation of the rainfall, runoff, and evapotranspiration processes for natural systems and engineered covers · Include evapotranspiration model for sparse covers and excess rainfall/runoff relationship · Include ability to deal with freezing conditions · Include vegetation growth models
Attenuation/retention	· Include representation of a range of sorption processes, using a variety of complex to simple K_d approaches, where applicable
Spatial heterogeneity and anisotropy	· Include representation of soil and rock features such as spatial heterogeneity and discontinuities
Degradation of engineering barriers, such as covers and liners	· Allow material properties to change over time for representation of degradation · Geomechanical representation of liner degradation through features like holes and cracks and processes such as oxidation, multi-layer surface cover degradation, and failure modes for both arid and humid environments · Allow for change in hydraulic properties with time
Radionuclide progeny	· Include representation of radionuclide decay chain products and differential transport of the progeny
Isolate performance of different engineering and natural features	· Need capability to identify relative contributions of different engineered and natural features as barriers that limit the impacts for a given problem, which will be used to 1) optimize design of remediation and disposal activities, and 2) to focus efforts on those aspects of the problem that are most significant in the context of the decision
Coupled processes	· Account for co-mingling of contaminant transport plumes · Account for mass transfer of contaminants influenced by physical, chemical, and microbial heterogeneities, and for biogeochemical influences on contaminant transport
Fractured media	· Include representation of discrete features which are currently modeled explicitly through mesh refinement or use of effective porous-media properties reflecting matrix and fracture contributions · Include fracture flow modeling to address cracking in concrete and grout, changing in fractures over time (degradation of concrete)
High ionic strength and osmotic potentials	· Represent osmotic potential in waste, function of water content

Table 5.1, continued

Area of Need	User Suggestion
Remediation approaches	· Represent remediation approaches, including: bioremediation through injection of reactive substrate or immiscible oils; in situ chemical reaction barriers; well models and representation of pump and treat systems (as many current codes lack features to effectively represent); unsaturated zone vacuum and passive extraction; and mercury transformation · Processes to represent in-situ remediation approaches are needed · Ability to represent in-situ processes in three dimensions and including reactions starts to justify the use of high performance computing
Coupled soil and hydrological processes with geophysics and isotope geochemistry for forward and inverse modeling	· Incorporate geophysical and isotope geochemical processes in the unsaturated-saturated media for improving forward and inverse modeling
Classification of Process Models	· Develop classification of process models, e.g., classification by areal coverage, types of geochemical processes, and types of modeling tasks · Develop integrated subsurface flow and transport simulators, including modular simulators for major types of contaminants, and simulators for the evaluation of environmental impacts of global climate change, water quality issues, sustainable remediation, etc.
Consider auto-parallelization	· Typically, parallel codes are designed to run on massively parallel machines, but this complexity is usually not needed; therefore construct codes with the intent to simplify parallelization

6.0 PERFORMANCE AND RISK ASSESSMENT REVIEW

To prepare for the ASCEM initiative, a preliminary review was conducted of codes and data used in recent performance assessments, and of composite analysis documents prepared in accordance with DOE Order 435.1 requirements. The review was conducted at the Hanford, Idaho, Los Alamos, Oak Ridge, and Savannah River sites. At these and other DOE-EM sites, performance assessment analyses are required to support waste disposal and tank closure actions, and risk assessments are conducted to support remedial action decisions. The objective of the review was to identify codes, methodologies, main assumptions, and key data.

6.1 Summary of Performance and Risk Assessment Codes

The ASCEM team identified a variety of codes and tools used in the performance and risk assessment process. These are summarized in *Table 6.1*. Few codes are commonly used at more than one site, but a number have common characteristics and functions (e.g. STOMP, PORFLOW, and FEHM). The codes range from relatively simple analytical

screening models to complex, multidimensional, multiphase flow and transport simulators. Each of the sites has developed the list of codes used in performance and risk assessment in consultation with the local regulatory agencies overseeing the work. (*Table 6.1* does not provide a list of utility codes since they are typically implemented to meet the needs of each individual site investigator and analysis.)

Table 6.1 Examples of codes used at major cleanup sites in the DOE EM Complex

Site	Code	References	Comments
Hanford	STOMP	White and Ostrom (2000; 2006) [15, 16]	Multiphase flow and transport code used for vadose zone simulations
	VAM3DF	Huyakorn and Panday (1999) [17]	Variably saturated flow and transport code used for groundwater simulations
	MODFLOW	Waterloo Hydrogeologic , Inc. (2005) [13]	Saturated zone flow and transport code used for regional groundwater simulations
	RESRAD	Yu et al. (2001) [14]	Radiation dose and risk code used to calculate dose and cleanup criteria
	MicroFEM	http://www.microfem.com Microfem (2009) [18]	Windows-based finite element groundwater modeling package for pump and treat design
Idaho	DUST-MS	Sullivan (1992, 2006) [19, 20]	Provides flux from waste form to the backfilled soil
	GWSCREEN	Rood (2003) [21]	Semi-analytical screening model for leaching and unsaturated, saturated transport
	MCM	Rood (2005a) [22]	Mixing Cell Model for 1-D transport in unsaturated zone under transient flow conditions
	MODFLOW	Harbaugh et al. (2000) [23]	Most recent INL regional flow model
	PORFLOW	ACRI (2000) [24]	3-D numerical model for unsaturated and saturated flow and transport
	RESRAD	Yu et al. (2001) [14]	Used to calculate intruder and radon doses
	RSM	Rood (2005b) [25]	Response Surface Model abstracted from MODFLOW results for transport in the Snake River Plain Aquifer
	TETRAD	Shook et al. (2003) [26]	3-D numerical model for multiphase unsaturated and saturated flow and transport
	CAP88	EPA (1990) [27]	Atmospheric dispersion and dose assessment

Table 6.1, continued

Los Alamos	HYDRUS-1D	Levitt (2008) [28]	Windows-based 1-D code for analysis of water flow and solute transport in variably saturated porous media, used to predict infiltration
	FEHM	Zyvoloski et al. (1995) [29]	Finite element heat and mass (FEHM) transfer code used to simulate groundwater flow and contaminant transport
	GoldSim	http://www.goldsim.com Goldsim (2009) [12]	Monte Carlo simulation software for modeling complex systems, used as platform for performance assessment simulations
Oak Ridge Reservation	TOPMODEL	Beven and Kirby (1979) [30]	Used in terrain analysis to incorporate topographic features into hydrologic modeling
	UTM	Patterson et al. (1974); Huff et al. (1977) [31, 32]	Unified transport model to simulate water budgets for surface and unsaturated zone water flow processes
	SOURCE1 and SOURCE2	Shuman et al. (1992); Icenhour and Tharp (1995) [33, 34]	Source release model for disposal units
	PADSIM and HOLSIM	ORNL (1997a and 1997b), App. D [35, 36]	Used to simulate unsaturated zone flow and transport: PASIM for above ground structures, and HOLSIM for underground waste units.
	MOC	Konikow et al. (1994) [37]	Method of Characteristics code used to simulate saturated zone flow and transport
	FTWORK	Faust et al. (1990) [38]	Block-centered finite difference model for simulating multi-dimensional flow and solute transport in saturated media under confined and unconfined conditions used to simulate saturated flow and transport
	Risk Analysis Calculations	ORNL (1997a and 1997b) [35, 36], App. D; USDOE (1996a) [39]; USDOE (1996b) [40]; USDOE (1991) [41]; USEPA (1989) [6]	Calculations completed using equations presented in performance assessments and following DOE and EPA guidance.

Table 6.1, continued

Site	Code	References	Comments
Savannah River	HELP	http://www.wes.army.mil/el/elmodels/helpinfo.html USACE (2009) [42]	Hydrologic evaluation of landfill performance code used to generate water infiltration estimates
	PORFLOW	ACRI (2000) [24]	3-D numerical model for unsaturated and saturated flow and transport used for flow and transport simulations in the vadose zone and groundwater
	GoldSim	http://www.goldsim.com GoldSim (2009) [12]	Monte Carlo simulation software for modeling complex systems, used for uncertainty analysis
	CAP-88	EPA (1990) [27]	Used to estimate annual dose

To address user feedback and the range of existing tools, ASCEM is implementing a graded approach for modeling that will enable analysis at varying levels of complexity. The features and processes embodied in many of the codes listed in *Table 6.1* are being incorporated into the requirements for the HPC Simulator thrust.

7.0 SUGGESTED TEST CASES AND DEMONSTRATIONS

During the user interview process, users provided input on test cases, datasets, or demonstrations that might address specific needs. *Table 7.1* provides a general view of that input. The ASCEM team will later determine if more information is required.

Table 7.1 User Suggestions for Test Cases

Process Need	Suggested Test Case, Dataset, or Demonstration
Nitric acid/ radionuclides/ metals/VOC plume	IFRC - Y-12 Plant S-3 disposal ponds
Uranium plume	IFRC – Old Rifle UMTRA Site, Colorado
Bioremediation	IFRC - Hanford 100 Areas
Uranium plume, interaction with Columbia river	IFRC – Hanford 300 Areas
Waste disposal above thick vadose zone	Hanford BC Cribs and Trenches
Surface barrier with extensive subsurface characterization	Hanford 200 Areas
Actinide migration from drums and concrete disposal shafts	LANL areas; MDA-G, MDA-L MDA-T, MDA-AB
Groundwater migration	LANL Cr Plume

Table 7.1, continued

Process Need	Suggested Test Case, Dataset, or Demonstration
Metals in soils	LBNL background soils characterization
Hg contaminated soils, surface and groundwater interactions; VOCs, DNAPL	Oak Ridge Y-12 Plant Integrated Facility Disposition (Hg SFA)
Burial grounds, deep well injection disposal, surface water and groundwater migration	Oak Ridge Melton Valley Watershed
Radionuclide and metals WAC development for PA	Oak Ridge Waste Management Disposal Facility
Dissolved phase DNAPL plume	Paducah Gaseous Diffusion Plant
PA Demonstration site	SRS Saltstone test plots
Seepage basins, acidic rad waste	SRS F Area
Moderator Leak (tritium point source)	SRS K Area
RCRA plumes	SRS A& M Areas, F&H Areas
Remedial alternative selection; pump and treat	LLNL 200 Site
Radionuclide fate and transport	NTS UGTA

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APPENDIX A. SUGGESTIONS FOR INTERVIEW TOPICS

Suggestions for Interview Topics
General Modeling/Regulatory Considerations
Are you subject to any regulatory directives/preferences regarding use of specific models, assumptions or data? If so, explain.
Examples of existing and upcoming modeling to support regulatory decisions: (need some examples of what is coming, but also need information about modeling that has been done)
- General description of the level of detail of conceptual and mathematical models (dimensionality, heterogeneity, discrete features, geochemistry, processes considered…) and names of computer codes.   - Do you use more detailed models to provide the basis for assumptions used for regulatory calculations?   - Specific ASCEM capabilities that would be useful for existing and future modeling efforts (e.g., reactive transport, fractures, stainless steel corrosion, concrete durability…) Examples of specific problems that would be supported, cost/significance? When are the capabilities needed (1 yr, 3-5 yrs, longer times)?   - Level of discussion should be sufficient to identify examples where the "Site Attributes" task may want to seek more detailed technical information.
- Engineered features considered in existing or future modeling (covers, vaults, tanks, activated metals, waste forms)?   - How is degradation or release from waste forms considered over time?   - How is degradation of engineered barriers (e.g., covers, vaults) considered over time?
- Remediation approaches considered in models (active remediation – vapor vacuum extraction, barriers or chemical treatment, natural attenuation, etc.).   - Do you have models capable of representing them?
Any recommendations for sites that would be useful for demonstrations for the Site Applications Task or data sets that could be used for testing/validation of specific elements of the ASCEM toolset?
Any specific capabilities that they would like to see in an ASCEM platform not captured above? (waste acceptance criteria, prioritize data needs, etc.)
Typical areas of interest for reviewers/regulators (examples of comments).
Data Management
Provide a list of databases used for site characterization data, research results, etc. (We are trying to identify sources of information that can be used for ASCEM).   - How are monitoring data maintained? Are monitoring data used as a comparison for modeling results?   - Do regulators have access to databases? Is there a need for databases that are publicly accessible or accessible to regulators only?

• In general: how are site characterization data, research results, and other information that would be used for modeling maintained (formal databases, spreadsheets, web access)?
Do you use automated tools to access information in databases during model execution? What features would be useful for such tools based on experience at your site?
What issues have you had passing information from one model or calculation tool to another? Did you develop automated tools to pre- or post-process information?
What is the typical level of detail for data used for regulatory calculations? (site specific or generic, spatial variability…) – (we are trying to get some feeling for the data availability relative to complexity of conceptual model)
• Example(s) of assessment(s) with extensive data.
• Example(s) of assessment(s) with sparse data.
What types of data management tools/capabilities would you like to see in ASCEM?

Visualization

How do you typically present results? (graphics, video, what information, etc.)
What tools do you use for visualization (e.g., TecPlot, GIS)? Are data stored in formats designed to be used for visualization?
Have any specific approaches to presenting results been especially effective with regulators/reviewers/stakeholders (video representations, specific types of illustrations)?
What visualization capabilities would you like to have in a new toolset?

Uncertainty Analysis/Decision Tools

How do you develop distributions for input parameters?
What tools do you use to conduct sensitivity/importance analysis and uncertainty quantification?
What process do you use to prioritize data collection for a given problem?
Do you believe that you are funding the most beneficial data collection activities or is there a need to be able to identify the most productive data to be collected?
Do you follow a specific approach to determine the level of detail to use for modeling a specific process within a given assessment?
Have your available models and hardware limited your options for conducting sensitivity/importance analyses and quantifying uncertainty? (have you had to simplify models used for Monte Carlo analysis)

APPENDIX B. SITE APPLICATIONS TEAM SUMMARIES OF RAW INTERVIEW DATA

GENERAL SUGGESTIONS

Need	User Suggestion
Effective integration of modeling and field activities	• Need to recognize that decision-making requires the efficient use of a combination of modeling, field sampling, demonstrations and other supporting activities. • The ASCEM tools need to help optimize the use of different resources in an efficient manner to support decisions.
Capability for regulators to use the toolset at some level	• Design the platform to have an interface that would facilitate regulator use of the tools, including executing simulations, "what if" analyses, and identifying key inputs and assumptions.
Security, firewall, and HPC hardware access considerations	• When considering data management in the ASCEM tools, need to recognize firewall and security restrictions regarding sharing of information outside of a given site. • Need to be aware of potential competition for time on HPC resources, especially considering tight schedules associated with regulatory calculations.
Learn from success of other codes	• Success of codes like RESRAD is due in large part to free availability. This encourages broad regulator use, involvement, and sponsorship during development and subsequent refinement. Free availability will help build familiarity and confidence in the tools' capabilities and accuracy. • One factor that helped MODFLOW's evolution was a single point of control during development and modification, which improved manageability. In addition, evolving a software package with a set of add-ons can decrease the transparency of the package and its capabilities, resulting in potential misuse or sub-optimal usage. MODFLOW is often misapplied, even though there are available training programs. • During their development, FEHM, NUFT, STOMP, TOUGH, and PORFLOW all grew and matured based on programmatic needs. For example, FEHM is based on a finite element approach, but can incorporate an orthogonal grid that can regularly and selectively subdivide elements into smaller sub-elements using an OCTREE approach. NUFT has a similar capability in its non-parallel version. Developers should consider the advantages of adaptive mesh capabilities that change with time.
Early demonstrations should include some simplified examples	• Need examples that illustrate the inclusion of the graded and iterative approach in the tools. Showing an early, simplified demonstration would reinforce the commitment to that concept.
Balance between ease of use and expert knowledge	• Need ability to balance between making the tools user friendly, and ensuring that users understand the problem being solved and how the tools can help address them. Ultimately, the tools have to be applied by knowledgeable users.

SUMMARY OF USER INPUT FOR PLATFORM THRUST

Data Management

Need	User Suggestion
Link to existing databases	Existing databases identified through end user interview process: • BIED/ERDMS (Savannah River Site) containing groundwater and analytical field data. Oracle based, internal web access • LANDMARK (Savannah River Site) geophysical log data • ArcMap (Savannah River Site) spatial geographic information system linked to BIED/ERDMS and LANDMARK • Groundwater monitoring in Oracle (Savannah River Site) to meet DOE Order 435.1 • ORES, PIMS, FMS may have useful systems and should be contacted (suggestions from Paducah Site) • Los Alamos Environmental Restoration Database (Los Alamos National Laboratory) • PHREEQ database, FEHM lookup tables for thermodynamic data (Los Alamos National Laboratory) • Oak Ridge Environmental Information System (http://www-oreis.bechteljacobs.org/oreis/help/oreishome.html linked with ESRI GIS platforms (Oak Ridge National Laboratory) • Database 4th Dimension, Version 6.05, ACI, Inc, Cupertino, California (Lawrence Berkeley National Laboratory) • Hanford Environmental Information System (HEIS – Hanford Site). Site contractor has initiated standardization of databases using Schlumberger's Hydrogeoanalyist, a comprehensive data management, visualization, and reporting package (will be integrated with HEIS). IFRC database is web-based with limited access currently, but will expand as project matures. Some data packages documented in reports (tank farms).
Model Data Input	• Current approaches consist of spreadsheets and text files for most applications. There are many software tools used to process data for model input in different components (e.g. bash, ksh, FORTRAN, NIX, MAKE, Excel spreadsheets, PERL scripts, and PYTHON). • Automated/batch data processing is necessary to 1) manage large numbers of simulations, 2) modify them in response to errors, updated inputs, and evolving needs, and 3) to maintain electronic records of the analysis. • Flexible tools are needed to read a process in different data formats. • Local data versus global data (e.g. thermodynamic databases) are managed differently, which leads to the challenge of how to translate local data in many different formats in order to model applications. • Local-scale data is often recorded in Excel spreadsheets. • It is a challenge to integrate information with different quality levels. • Connections to GIS tools are useful. • Connection with existing Groundwater Modeling System (GMS) tool is useful. • It is important for the user interface be designed for "informed" users rather than for a general audience.

Summary Input for Platform Thrust, Data Management, continued

Data Integration	• Need data reviewer/format tools for easier interoperability between databases and models. • Need improved ability to link information from different sources within a GIS framework. • Need approaches to optimize field data and process understanding in combination with modeling. • Need to address access and firewall considerations at most DOE sites.
Error checking	• Transferring information between different modeling components is a frequent source of errors due to the volume of information being processed. • It is difficult to make changes for an input parameter (e.g. for sensitivity/uncertainty analysis) and ensure that all related parameters are updated appropriately. • Need traps for input data errors. • Dealing with conceptual model errors is a large challenge.
Database Maintenance and Usability	• Yucca Mountain Project database may be an end member type example for database maintenance and usability.
Data Abstraction and Transfer Between Codes (data input)	• Need to resolve issues regarding passing information between models. The example given was between FEHM and Goldsim. ASCEM will face the same issue.
Borehole Data	• Need the ability to enter borehole data into the system and integrate it into geologic conceptual models.
Data Tracking and Provenance	• It is important to track data to original sources and maintain transparent representation of input data for specific aspects of a problem (graphically would be ideal). • Need to be able to propagate change in one input variable through different components and dependent parameters. • Need the ability to track changes in applications and generate logs.
Regulators expect transparency and traceability	• Interfaces with databases need to consider regulator expectations for transparency and traceability of inputs and assumptions, as well as facilitate easy access to key information. This will be closely tied with conceptual models.
Link results with need to develop monitoring plans, data quality objectives, waste acceptance criteria	• Consider structuring database to have specific reports that will facilitate the development of monitoring plans, monitoring reports, development of data quality objectives, and other expected needs.
Archival and passing on to LM	• Need the capability to maintain information regarding key assumptions and requirements. This information sometimes must be passed to Legacy Management or, similarly, it will be used for the development of a facility's waste acceptance criteria and operational controls.

SUMMARY OF USER INPUT FOR PLATFORM THRUST

Conceptual Models

Need	User Suggestion
Regulators expect transparency and justification of assumptions	- Data used for the development of conceptual models need to provide calibration targets: simulations best fit to data. - Development of conceptual models to provide results that may be used in the regulatory decision process (e.g., CERCLA). - Many regulatory analyses require simplified calculations, and abstractions from complex data are often performed. - The ASCEM Platform needs to assist the regulatory process for treatability tests and feasibility studies. Specifically, ASCEM needs to consider Data Quality Objectives and the Sampling and Analysis Plan process. The open-source aspect of the Platform and HPC will be useful for regulators to openly participate in the development process. Specifically, it will be useful for dealing with the many explicit decisions made during the modeling process and in identifying data gaps. - Need a graded approach to modeling. Less complex approaches will be needed for regulatory documents. A structured output that provides pedigreed data will be useful. - Need a common conceptual model platform for regulators to review so that data gaps are identified early.
Propagation of changes in dependent or similar data that appear in multiple modules for a given realization/simulation	- Need the capability to automatically propagate changes in parameter values or assumptions in one module to similar or dependent parameters/assumptions in other modules used for the same realization/simulation. - Data examples: saturation profiles; porosity; contaminant concentration; lithology; permeability; and geochemistry.
Screening tools to eliminate pathways, radionuclides, etc. of minimal significance	- Need to eliminate insignificant pathways, processes/features, and contaminants from conceptual models. Conceptual models should reflect the necessary level of complexity (i.e., consider dual continuum, some discrete features and processes) to provide 1-D, 2-D, or 3-D simulations/predictions. - Need the ability to defensibly prioritize data needs in order to limit the need to collect large amounts of field data that may not have a significant impact on a decision.

Summary Input for Platform Thrust, Conceptual Models, continued

Need	User Suggestion
Multiple sources and processes at multiple scales over large areas	• Couple many processes: multiphase; dual continuum; multi-component reactive chemistry; heat (non-isothermal); colloid model; coupled atmospheric/watershed/infiltration; and robust water table model. • Provide detailed conceptual models for each watershed and specific sites within the watershed, including: surface hydrology; geohydrology; geophysical; meteorology; chemical and radionuclide surface water and groundwater transport; geochemistry; microbial and pH influences on contaminant mobility; SW/GW interaction and shallow GW flow; and fractured flow. • Recognize a time dependent behavior of K_ds and solubilities of contaminants. • Provide models of hydraulic isolation of waste disposal areas that serve as the source for contaminants. • Provide conceptual models to better understand subsurface processes influencing migration, prioritize single sites and integration points for remedial action, and support development/ implementation of remediation technologies. • Provide conceptual models for near term assessments of deep subsurface migration of contaminants to potential off-site locations to determine the extent of migration. • Provide conceptual models to describe degradation or release from waste forms over time, including release of hazardous constituents, radionuclide progeny, and chemical degradation products. These models need to support the regulatory compliance timeframes and individual, single site remediation actions, as well as remediation actions at watershed integration points. • Use a systems analysis approach in developing conceptual models. • Provide conceptual models to simulate failure scenarios that follow best engineering practices and local and federal regulatory guidelines. They can also be used for regulatory scheduled remediation actions.
Development of waste acceptance criteria	• Need the capability to back-calculate acceptable source loading (concentration, inventory) linked to a dose or risk endpoint. This will need to be radionuclide- and waste form-specific, including debris, soils, metals, and cementitious materials, etc. • It would also be useful if the tools could represent time- and space-dependent waste loading into a facility to provide more resolution, which is useful in assessing waste acceptance on a real time basis (quick turnaround).

Summary Input for Platform Thrust, Conceptual Models, continued

Need	User Suggestion
Recognize need to use proper tool to solve each problem (graded and iterative)	• Models need the ability to mix and match capabilities as appropriate to the question being addressed. • Models should be neither too simple, nor too complex. An example of an overly simple model involved a Tier 1 analysis incorrectly predicting a very long travel time of Cs from a waste tank to the water table due to sorption of the Cs. A more complex model that included competition for sorption sites by multiple ions showed that much of the Cs was not sorbed. Regulators often require performance confirmation data collection in order to compensate for such situations in which the model does not address the correct question, unbeknownst to either the applicant or the regulator.
Waste isolation/containment technology evaluations	• Need to support better assessments of waste isolation and containment technologies in diverse/complex environmental settings, including: barriers; vaults; encapsulation; covers; liners; containers; repository; etc. This is particularly true of *in-situ* technologies.

SUMMARY OF USER INPUT FOR PLATFORM THRUST

Uncertainty Quantification

Need	User Suggestion
Need to develop a catalogue of methods for the uncertainty analysis, including	• Need a decision tree to provide guidance for choosing an appropriate uncertainty analysis method for decision-making under uncertainty, including experimental/measurements/design uncertainty assessment, modeling uncertainty, risk assessment. • If reliable estimates of probability distributions cannot be defined, it may be more useful to proceed with uncertainty analysis on the basis of bounds on sets of probability distributions, interval analysis, fuzzy systems modeling, sensitivity analysis, or to use Generalized Likelihood Uncertainty Estimation (GLUE), Bayesian methods, expert elicitation, etc.
Computing limitations impact ability to conduct full probabilistic uncertainty analysis	• Need efficient uncertainty analysis capability to conduct more quantitative uncertainty analysis for higher complexity models (i.e., multiple realizations of complex 2-D or 3-D models, refined mesh, and reactive transport).
Similar and dependent input data and parameters may be present in different modules/models, all values need to be updated consistently if any one is changed	• Need to consider approaches to reducing modeling uncertainties through identifying and tracking similar and/or dependent variables that are present in multiple modules/models. This would allow all to be consistently updated in Monte Carlo (or other methods of the uncertainty analysis) realizations.

Summary Input for Platform Thrust, Uncertainty Quantification, continued

Need	User Suggestion
Decision makers and regulators need to be able to understand results and identify key aspects of the problem (linked with decision tools)	• Consider approaches for illustrating/presenting results of uncertainty analyses and sensitivity (importance) analyses in layman's terms. Identify significant contributors to uncertainty (such as experimental uncertainty and modeling uncertainty), which could potentially impact predictions, risk assessment, cost, and selection of remediation methods. • In the uncertainty evaluation, distinguish the effect(s) of features and assumptions from the effects of sensitive model parameters. • Distinguish sensitive parameters that, when changed, have a significant impact on the conclusions from those sensitive parameters that may significantly affect predicted doses, but not to the extent that conclusions would change.
Uncertainty in conceptual models, failure scenarios, etc. and also effectiveness of different remedial actions	• Need tools to quantify the influence of assumptions regarding the choice of conceptual models for specific features, events, or processes, such as failure modes for engineered barriers or waste forms. • The tools should also be capable of identifying the relative importance of different barriers (e.g., waste form, container, vault or tank, vadose zone, etc.) in terms of the eventual dose that is projected. NRC refers to this as "barrier" analysis. This can also apply to the effectiveness of different remediation technologies.
Importance of parameters and assumptions will change depending on point in space and time	• Need the ability to separate out parameters that are important for early peaks from later peaks (due to different radionuclides). • Importance is a function of time. • Also, sort out importance as a function of location of dose for situations with multiple source terms that discharge to different receptor locations. Tank PAs have shown that parameters that are important for a dose at one location resulting from releases from a specific tank are not the same as the parameters that are important for peak dose at another location that results from a different tank.
Aleatory and epistemic uncertainties	• Need to be able to take into account both aleatory and epistemic uncertainties in order to reflect their relative importance in the context of the problem being solved. • It is of interest to identify reducible uncertainties so that appropriate site characterization, monitoring methods, or field demonstrations can be designed for the data collection, as well as for the selection of appropriate conceptual and numerical models.
Uncertainty analysis with two- and three-dimensional models	• Include distributed processing and computational efficiency to enable probabilistic analysis in full physics mode.
Improved tools to support uncertainty/sensitivity of design failure analyses	• Need uncertainty and sensitivity analysis tools to support design failure scenarios for engineered waste isolation technologies or storage facilities.

SUMMARY OF USER INPUT FOR PLATFORM THRUST

Decision Tools

Need	User Suggestion
Graded and iterative approach	• Need a robust approach for identifying and prioritizing areas requiring more detailed consideration as the iterative process proceeds. • Need tools that use results of increasingly complex models to prioritize areas where increased complexity is expected to provide the most benefit, considering model sensitivity/uncertainty and data collection needs. • Need decision-making to support the iterative modeling approach (which identifies critical data needs and areas where increased modeling complexity would be expected to provide the most benefit regarding decision to be made). • Need methods for abstracting results from complex models for use in decision-making tools
Systems analysis, cost/benefit, decision analysis	• Implement systems risk analysis tools to support decisions concerning potential D&D and technical project risks during environmental restoration. • A systems analysis approach could be employed in which bounds of known and suspected contaminated media and potential high risk transport pathways could be documented using geographic information system (GIS) technology, and ranked according to risk. This information would be used to identify areas that would benefit from further site reconnaissance. • Where appropriate, a comprehensive three-dimensional subsurface model of fluid flow and reactive chemical transport, focused on contaminant pathways, could be utilized to evaluate and predict the impact of D&D activities and remediation actions. • Use of the model could improve the efficiency and cost effectiveness of remediation, and reduce overall technical risk and uncertainty. • Information gained from the use of this systems analysis approach would also increase understanding and contribute to the development of cost-effective groundwater remediation decisions for final RODs. • Need to have cost/benefit analyses performed along with technical implementation and performance evaluations. • Need a tool for decision analysis that identifies parameters that result in failure scenarios. • Need cost/benefit analyses conducted to support remediation actions and associated sampling.

Summary Input for Platform Thrust, Decision Tools, continued

Need	User Suggestion
Integration and Optimization of Data collection, Monitoring, remediation system design and modeling	• Need a comprehensive subsurface modeling tool and monitoring system to evaluate the effectiveness of the remediation actions, and facilitate decision-making on final actions. • Need a comprehensive monitoring strategy and system to determine the optimum type and placement of sensors and monitoring points to assess the condition of ground and surface water before, during, and after remediation. • Interim assessments and modeling results will reveal situations appropriate for remediation technologies. • Need to optimize cleanup/closure strategies across a site. • For better decision-making, it is necessary to optimize data collection and modeling complexity. • Need approaches to optimize use of field data and process understanding in combination with modeling. • There is a similar need for the ability to defensibly prioritize data requirements to limit the collection of large amounts of field data that may not have a significant impact on a decision. • Sampling optimization techniques are utilized for frequency of sampling events, number of samples, and locations of samples. • Need to consider prioritization of data collection, for example using Adaptive Management Approach in conjunction with EPA's Stressor Identification Process. • DQO process has proven effective using sensitivity analysis, process knowledge, and regulator interest. • Need cost/benefit analysis with respect to data collection activities and the data's potential influence on the EM decision.
Field test/treatability test design	• Include design analysis for conducting field tests (e.g., rates, concentrations, etc.). It will assist with the regulatory process for treatability tests and feasibility studies.
DQO optimization/identification of data gaps (transparency with regulators)	• The open-source aspect of the Platform and HPC will allow regulators to openly participate in the development process. Specifically, it will be useful for dealing with the many explicit decisions made during the modeling process, and help to identify data gaps. • Need to allow non-experts to quickly identify key assumptions. • Regulators see models as black boxes. Need tools that facilitate transparency and confidence building with respect to model results. • Need to adopt DQO process along with a model specific QA/QC plan that specifies the use of model and modeling results.

Summary Input for Platform Thrust, Decision Tools, continued

Need	User Suggestion
Conceptual model testing/optimization tools	• Need the ability to conduct parallel assessments using different conceptual models or assumptions for specific processes or barriers in order to compare how assumptions can affect conclusions. • Need the capability to conduct barrier analyses to identify and quantify the relative impacts of different barriers and failure scenarios on overall performance. • Also need the ability to test different design concepts. • Conceptual models, coupled with model testing and iterative model development, generally provide the best means of determining data needs.
Uncertainty analysis/sensitivity analysis/model abstraction evaluation	• Need to enable uncertainty analysis with more complex models (3D, 2D) in order to evaluate impacts of abstractions. • Need tools that enable communicating the sensitivity of results. • Need guidelines and structured approaches for conducting probabilistic assessments, including appropriate methods of abstraction and sensitivity analysis. Regulators remain interested in deterministic analyses to address "what-if" questions.
Optimization tools to support technology selection and implementation	• Need optimization tools for watershed and composite analysis coupled with uncertainty/sensitivity analysis tools.

SUMMARY OF USER INPUT FOR PLATFORM THRUST

Risk Assessment

Need	User Suggestion
Integration of environmental monitoring data with models	• Need better coupling of monitoring data with modeling to assess remediation effectiveness (risk reduction) at regulatory compliance points for surface water and groundwater. • Need better data management, analysis and visualization tools for integration.
Better understanding of Hg fate and transport	• Need capability for modeling fate and transport assessment of environmental forms of Hg and exposure assessments for ecological and human health endpoints. • Need modeling to support understanding of microbial and geochemical influences and reactive transport of Hg.
Address processes associated with surface exposures	• Need to address surface interactions associated with intrusion scenarios (transport and exposure via flora and fauna that come into direct contact with waste or radionuclides, uptake in plant roots, erosion, resuspension, dust loading, etc.). The number of processes that could be considered for these pathways and scenarios is often site-specific and can multiply quickly, so it will be important to prioritize efforts in this area.

SUMMARY OF USER INPUT FOR PLATFORM THRUST

Visualization

Need	User Suggestion
Illustration of importance and uncertainty quantification	• Need visualization tools to conveniently present uncertainty quantification-related results of simulations, as well as specific plots to support importance analysis for input parameters and assumptions (3-D surfaces to illustrate responses for multiple parameters, scatter plots, influence diagrams, etc.).
Animations are very effective with decision makers and regulators	• Need animations to show evolution of a problem over time (moisture, redox, concentrations, etc.). Sliders were mentioned as an effective means of illustrating how changes in specific inputs influence results. • In general, there is a need to plot nodal distributions of key variables and assumptions and illustrate changes over time.
Reality checks and quantification of significance of different "barriers"	• Need the ability to plot intermediate results (flux to water table, release from source term region, performance of specific "barriers" in the system) to help understand system behavior. This supports the ability to conduct "barrier" analyses.
Mesh and input development tools	• Need visualization tools to debug assignment of material properties in a mesh and quickly show reviewers material properties for a specific region.
Plot data and derived distribution together (NRC preference)	• Need the ability to plot derived distributions and empirical data on the same graph (process for developing distributions) to illustrate the relationship between what you know and what you are assuming.